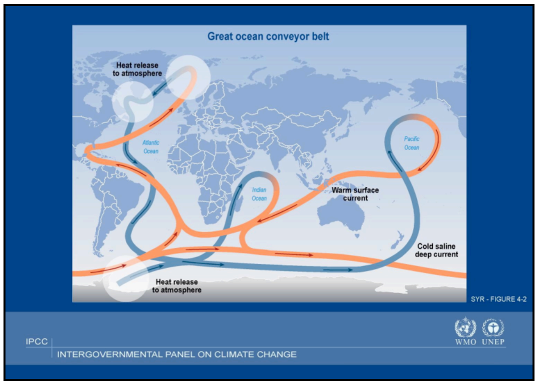
CCS News Bytes

LALP-05-015 March-April 2005



This illustration shows how warm water flows to the north and cold water sinks to the bottom and flows south on our planet. It can take 1,000 years or more for water to complete one circuit.

Ocean Modeling: a Step toward Understanding the Earth's Climate

Matthew Hecht and Beth Wingate are working on two massive, interlocking problems with thousand-year time scales: ocean and climate modeling.

In a recent interview, Hecht, a staff member in CCS-2, the Continuum Dynamics Group in the Computer and Computational Sciences Division (CCS), said, "Much of ocean modeling is geared to climate (not weather)." He added, "Here, we also have specialized in shorter-term, very detailed simulation of ocean circulation."

Atmospheric modeling is complex, but ocean modeling presents a broader range of time and space scales. The oceans also store much of the available heat in the climate system. "There's just a lot more material in the ocean than in the atmosphere," Hecht commented. Going down just 10 meters below the sea surface doubles the pressure felt at the surface, because there is as much mass contained in 10 meters depth of water as in the entire column of air above. The ocean is essential to understanding climate not only because of its role in the heat budget, but also because it holds much of the Earth's available carbon. The ocean's role as a source or sink of carbon dioxide to or from the atmosphere is determined primarily by water temperature.

The Rise of POP

In CCS, five staff members and two postdoctoral researchers are working on ocean simulation. Wingate, a staff member in CCS-2, said the cornerstone of ocean simulation is the Parallel Ocean Program (POP). She said it exists because of Bob Malone, a now-retired CCS-2 group leader. He saw an opportunity to take the best ocean model that existed at the time and make it work on massively parallel computers.

Malone is "a hero of nuclear winter," Wingate commented. He developed the "Nuclear Winter Prediction Model." He knew a lot about modeling of the atmosphere, she said—but he also had the insight to realize that if the work were done right, a smaller number of people could study ocean modeling successfully.

(Please see OCEAN, page 3.)

EpiSimS Featured in *Scientific American*

It's not every day that the Computer and Computational Sciences Division (CCS) has a feature article in *Scientific American*.

Placing an article about EpiSimS in the March 2005 issue of the magazine was a major accomplishment. In a recent interview, James P. Smith, leader of the Discrete Simulation Science Project (CCS-DSS) and one of the co-authors of the article, described the process of preparing the document and the impact of its publication.

What Is EpiSimS?

EpiSimS is a computational tool that makes it possible to simulate the spread of diseases such as smallpox or anthrax at the level of individuals in a large urban setting. It takes into account realistic contact patterns and disease

(Please see EPISIMS, page 2.)

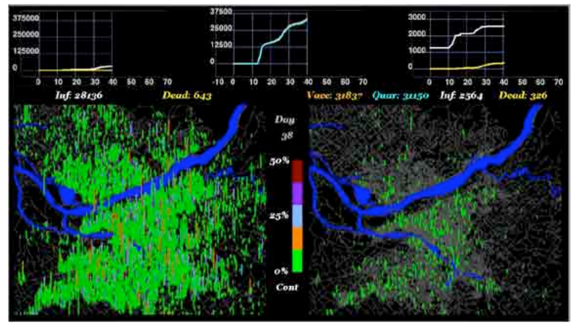
EPISIMS (Cont'd from P.1.)

transmission characteristics and provides estimates of the geographic and demographic spread of the disease over time.

It can be tailored to reflect the nature of individual activities—revealing, for example, the transmission rate of the disease among elementary school children in a classroom as compared with the same children on a soccer field or adults in offices.

Because EpiSimS provides detailed and accurate estimates, urban officials could use it to simulate the spread of disease in a crisis and then select among methods for fighting the epidemic—methods such as quarantines, vaccinations, or the use of antibiotics.

EpiSimS takes advantage of human mobility information derived from TRANSIMS, an earlier Los Alamos National Laboratory tool that estimates the movement of people as constrained by transportation infrastructure. TRANSIMS is based on census data and activity surveys taken from a small sample of the population in a particular city.



These two EpiSimS images show the simulated effects of different approaches to fighting an imaginary outbreak of smallpox in a particular American city. The image on the left shows the impact of the epidemic 35 days after the initial outbreak if no public health intervention is undertaken. The image on the right shows the effect if infected and exposed individuals are vaccinated and quarantined. A series of simulations showed that the most effective strategy under these circumstances would be to have people withdraw to their homes early in the epidemic.

Contact with the Magazine

Smith said that *Scientific American* actually requested the article.

"Their editors apparently attend prestigious science meetings and try to identify topics appropriate to their audience," Smith said. In this case, an editor made contact with Stephen G. Eubank during a meeting of the American Association for the Advancement of Science. (Eubank and Chris L. Barrett, the other two authors of the article, were technical staff members in CCS-DSS at the time. They have since left the Laboratory.)

Eubank returned to CCS-DSS with the news, and the team began work.

"I wrote the first draft," Smith said. "We actually made our deadline"—a surprising experience for the editor. The initial article was about 4,500 words long with five pages of illustrations, diagrams, and figures.

The magazine, however, wanted a 3,000-word article.

"We made a second try that was a little longer," Smith said. Then a *Scientific American* editor, Christine Soares, took over. Smith said, "She took this 50%-over article and made it into something that fit and was better. It was an amazing experience. There was not a single thing she did that wasn't right."

The three co-authors made a few minor changes, finishing just a few weeks before the March issue of the magazine came out in February. All in all, the process took nine months.

Response to the Article

Asked about his reaction to the article, Smith said, "I thought it was great," and, he added, the response has been "really good."

He said, for example, "Some university professors have asked to use the materials in teaching." And he has received perhaps a dozen e-mail messages from interested people ranging from elementary-school children to adults with a variety of backgrounds.

One child who enjoys playing a city simulation video game wanted to know if there might be an EpiSimS add-on. Smith noted that to simulate a large metropolitan area, EpiSimS requires a 200-gigaflop computer with 200 gigabytes of RAM—well beyond the capacity of a typical child's gaming platform.

On a more serious note, Smith said, "Several exciting new professional connections have come out of this article."

(Please see MORE EPISIMS, page 6.)

OCEAN (Cont'd from p.1)

Hecht said ocean modeling doesn't require as many people because oceans do not have clouds—pesky structures that pose microscopic issues that constitute a very large problem in atmospheric modeling but cannot be ignored.

Wingate said the POP people in T-3, the Fluid Dynamics Group of the Theoretical Division (John Dukowicz and Rick Smith, at the time) "took the world's best model and made it run fast on parallel computers. Then, they started developing their own model."

Wingate added, "We also are working on new models."

Hecht does massively parallel, high-resolution calculations on the big machines at the Laboratory. He is also doing next-generation models. The products of his work are voluminous files of data, which can be analyzed to find out important things about ocean circulation or global warming. He also produces pictures that are a visualization of the data.

The North Atlantic Model

Wingate has a Ph.D. in atmospheric science and scientific computing from the University of Michigan. Hecht has a doctorate in theoretical particle physics "with a computational bent" from the University of Colorado-Boulder. He commented, "I didn't even think to study climate until I went to a seminar." A light bulb came on in his head that day, and he did his postdoctoral work in ocean modeling. Both of them have a background that includes work at the National Center for Atmospheric Research in Boulder.

Hecht was a postdoctoral researcher at the Laboratory between 1995 and 1997 when he worked with Rick Smith and Matt Maltrud in T-3 to develop a North Atlantic model. Hecht said, "It was a breakthrough simulation in terms of getting the most realistic picture anyone had seen of the Gulf Stream."

"You never really know if your model is sufficient until you do it," he commented. At the time, it was not known what resolution was required, nor whether the model physics was sufficient to achieve a realistic simulation of the Gulf Stream.

Wingate said that the effort for them to get a realistic picture of the Gulf Stream was as expensive in terms of memory as the entire coupled climate model. Hecht added that it was bigger than anything others were running at the time. He said they did it on the CM5 Connection Machine in the Advanced Computing Laboratory, headed at the time by Andy White, who had the necessary computing resources from the Department of Energy (DOE) Office of Science.

Recent Work

Hecht added, "More recently, we've been working to figure out how to model climate with an eddy resolving ocean." Maltrud, he said, is doing a global ocean-only simulation.

Wingate said their work involves a multidirectorate team with people from the Atmospheric, Climate, and Environmental Dynamics Group (EES-2) as well as T-3 and CCS-2.

Hecht added that their work is part of the Community Climate System Model. At one time, the ocean component was based on a National Oceanic and Atmospheric Administration model, not the Laboratory's DOE model (the POP code). Malone, Wingate said, was, "the captain who made everything possible on the ship."

The model is showing global warming. Hecht and Wingate said, "It's still a little bit of a judgment call" as to whether warming of this scale is man-caused or natural, but Hecht added, "It's a bit of a stretch (now) to see the warming of the last three decades as natural." They said that research on everything from tree rings to ice cores is indicating that the human race has created the problem. Hecht noted that the current retreat of ice is of particular concern. Because the ice is melting, he said, "The planet—like a black wall—is soaking up more sunlight."

Hecht's work on the Gulf Stream shows how relatively warm, salty waters feed into an area where dense waters are produced in the North Atlantic. Warm water flows to the north at the top of what has come to be called the Great Ocean Conveyor Belt. Cold water sinks to the bottom and flows south. "You're taking heat north," Hecht said. "The question is, how cold are those returning waters?"

It can take 1,000 years or more for water to complete a circuit of the conveyor belt.

Wingate is working on "overflows" in collaboration with the larger scientific community. She is looking at how dense water goes down the "slope" to the bottom, a process which, Hecht says, "we need to parameterize."

An Office of Science document, "Multiscale Mathematics Initiative: A Roadmap," published in December 2004, noted that breakdowns in this circulation pattern have in the past been associated with rapid climate changes.

(Please see MORE OCEAN, page 6.)

Meet Our New People

Two new technical staff members recently joined the Computer and Computational Sciences Division. Brief biographies of each of them appear on the next two pages. Please make them welcome!

Mark A. Christon

Mark A. Christon, who joined the Continuum Dynamics Group (CCS-2) in the Computer and Computational Sciences Division on January 31 as a technical staff member, holds a bachelor-of-science degree, a master's degree, and a doctoral degree in mechanical engineering from Colorado State University in Fort Collins, Colorado.

He brings with him significant experience from two other national laboratories.

He spent five years as a technical staff member at Lawrence Livermore National Laboratory, working in the Methods Development Group. He worked on codes for acoustic fluid-structure interaction; on time-dependent incompressible fluid flow; and, "a little," on DYNA3d, a code for simulating Lagrangian dynamics.

He then moved to Sandia National Laboratories in Albuquerque, where he worked for about 10 years, primarily in incompressible fluid flow. He also worked on the ALEGRA code, doing Lagrangian and Eulerian shock hydrodynamics.

During his time in Albuquerque, he closely followed the work done in Los Alamos by such scientists as Doug Kothe, Bill Rider, Gary Dilts, Larry Libersky, and others. Christon also interacted with them at conferences.

He was attracted to CCS by "the group, the work, and the reputation," he said. "I've wanted to be up here for a long time." He was especially interested in the Telluride Project (which can be used to simulate many problems in the areas of solidification, fluid flow, heat transfer, phase transformations, and mechanical deformation) and the Marmot Project (a component-based hydrodynamics effort)—and he is now working on them. "The people are just tremendous here," he said.

Christon is married, and his wife, Elisa, is a third-grade teacher. He has two children, Jennifer, a high school junior, and A.J., a sixth grader. For the time being, he is commuting from Albuquerque to Los Alamos, while he works on selling the family home and preparing to move. He hopes that his daughter will be able to finish high school in Albuquerque.

Because he is commuting, he has relatively little spare time. He has been doing a combination of driving, riding the bus, and telecommuting, and he is looking into airplane pools and vanpools.

He said he spends the spare time he has with his family. "I like to ride dirt bikes with my kids," he said. He also likes to ski and has already taken his family to Pajarito Mountain Ski Area "a time or two." He is also very involved with his son in Boy Scouts. They recently camped together in the snow at Hyde Park near Santa Fe.

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John Wohlbier

John Wohlbier has a bachelor's degree, a master's degree, and a doctoral degree in electrical engineering from the University of Wisconsin (UW) in Madison, Wisconsin.

He also has experience in private industry, and he once ran his own company.

After he earned his bachelor's degree, he worked at a startup company in Middleton, Wisconsin, called "Soft Switching Technologies." He had many different assignments during his time with the company, doing mechanical design on a set of electroplating power supplies, doing production management, and doing some programming of field-programmable gate arrays, among other things.

"At the same time," he said, "I was running my own company," Jaksound, which was "a sound-reinforcement company," providing public address systems for bands and other uses. Wohlbier was (and is) a musician in his spare time. He has played both drums and guitar, and at one time, he had a rock band, "Seize Mars," that played for clubs.

He returned to UW to earn his M.S. and Ph.D., and then did postdoctoral studies at UW in the Engineering Physics Department. His postdoctoral research was in fusion. He said he worked on ballooning modes in the stellarator, a fusion device.

Wohlbier came to Los Alamos National Laboratory in September 2003, joining NIS-10 (subsequently International, Space, and Response-10 and now ISR-6, the High-Power Electrodynamics Group) as an engineer/physicist. His work there involved theory and computation of microwave vacuum devices.

He was attracted by the computation and hydrodynamics work being done in the Continuum Dynamics Group (CCS-2), and eventually answered a CCS-2 job ad that looked interesting. He changed groups this year.

He is now doing hydrodynamics work involving the RAGE Code—in tight partnership with the Applied Physics Division (X Division). There are three people in CCS-2 on a hydrodynamics team now deployed to X Division, and Wohlbier is one of them.

Wohlbier and his wife, Piper, have two daughters, Evelyn, 3, and Lorelei, 16 months old.

He said he spends most of his spare time with his family. He has a wide range of interests. He is a runner (and recently signed up for the 13-mile Pike's Peak event for the second year in a row); he is studying jujitsu (a Japanese martial art); he still plays the guitar for his family; he likes skiing and has already taken the family to Pajarito Mountain Ski Area; and he also enjoys cooking.

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Forslund Is Back at CCS after a Brief 'Retirement'

Dave Forslund retired from the Computer and Computational Sciences Division (CCS) in June 2004 after more than 35 years at Los Alamos National Laboratory (LANL)—but now he's back. Actually, he never stopped working.

In a recent interview, Forslund, a LANL Fellow, said, "My job was interfering with my work. I didn't retire to stop working. I continued to work on my own. A lot of what I did as a Fellow was like that anyway."

What Drew Forslund Back

So why did he come back?

"I think the Lab is an extreme value to the nation," he said. He wants to help it succeed. He commented that LANL "holds knowledge that isn't anywhere else." He likes to stay ahead of the scientific curve, he said, thinking of important things before others notice them, helping people to see things, and helping them benefit from his historical knowledge.

He has been paid since November 2004, but he can only work 40% of full time. The result, he feels, is that he can make a contribution, but he never has to work excessive overtime—no matter who is asking.

Current Work

He is working on two projects right now.

One involves the Nuclear Materials Technology Division.

The other is the Biological Warning and Incident Characterization Project (BWIC), sponsored by the Department of Homeland Security. BWIC involves Sandia National Laboratories, Argonne National Laboratory, Oak Ridge National Laboratory, Lawrence Livermore National Laboratory, and Pacific Northwest Laboratory, as well as LANL. LANL's major responsibility in the project is "public health surveillance and modeling."

BWIC

BWIC's goal, as Forslund described it in a recent PowerPoint presentation, is to "develop a robust, integrated, biological warning and incident characterization decision-support system, which facilitates timely warning, attack assessment, and effective response in the event of a biological attack."

BWIC seeks to combine information from biosurveillance and environmental monitoring systems with key modeling tools and databases. The goal is to integrate the nation's environmental monitoring data (from such things as the BioWatch detectors that sniff the air for potential bioagents) with public health surveillance information (from hospitals, emergency rooms, pharmacies, and school and business absenteeism records) so that officials know how to respond if they are facing a biological "event." He said the project will link up with "epi-modeling." It will even include data sources such as urban meteorological information. When all of these capabilities and sources of information are in place, officials facing a biological emergency should be able to predict what will be happening within 24 hours—and make the best possible decisions.

Forslund noted that he was involved in the Biodefense Initiative in Albuquerque in 2002, which involved work with hospitals, an ambulance service, and others. BWIC is "sort of a follow-on," he said. "I'm basically an expert from the architectural point of view." In addition, he has been working with the New Mexico Department of Health for almost a decade and still provides consulting advice on request.

In an era in which the United States population could face deliberate terrorist threats to release smallpox and anthrax, BWIC could prove to be a tool of major importance to the nation.

Some Thoughts on LANL and Retirement

Forslund said he also hopes to play a role in helping the Lab decide what to do with retirees. His own philosophy is that the Laboratory should encourage retirees to come back as mentors who can transfer knowledge to the younger staff members. Such mentoring work should be both required and paid, he said.

He feels that the Laboratory must address morale first if it wants to achieve its complex goals.

He has worked under every Laboratory Director since J. Robert Oppenheimer (and he was at Princeton with Oppenheimer). He remembers a day when many things were done differently. He mentioned that, "(Then-Laboratory Director Harold) Agnew would just drop in on your meetings—unannounced."

(Please see FORSLUND, page 6.)

FORSLUND (Cont'd from P.5.)

He said former Laboratory Director Sig Hecker made heavy use of the Science and Engineering Advisory Council, sharing information about his problems with SEAC members and making good use of their comments on technical and morale issues.

Forslund recalled that when he first arrived from graduate school in 1969 (with a Ph.D. in astrophysics from Princeton and a plan to "be here two years and move on"), he encountered a very effective training system.

The first week, he said, he was provided with a crash course in "nuclear physics for everyone." The second week, he was taught "the basics of bomb design for the technical staff." The third week, he was given a tour of "every single experimental laboratory facility this Lab had."

He said the process "convinced me that this Lab was very important and unique … vitally important to the nation."

As a result, he never left.

"If I had spent the first two weeks doing ES&H (environmental, safety and health) training, I don't think I'd be here today," he said. Those things are very important, he emphasized—"but you've got to set your priorities."

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MORE OCEAN (Cont'd from P. 3.)

The document said, "Similarly, the rapid warming we are currently experiencing could trigger an abrupt thermohaline shutdown and subsequent regional cooling. Numerical solutions have revealed that incorrectly predicting the 3d turbulence of the Kelvin-Helmholtz mixing can cause drifts after only 100 years of a 1000-year-long ocean simulation. In the Primitive Equations of motion that are used by most climate researchers worldwide, the small-scale phenomena are not included. If we continue with current models, then as computers get larger and as resolution increases, we will still not capture the phenomena described above. Instead, the processes are approximated by local empirical models that have to be changed with the changing resolution of each model run. Overflows could be resolved with a brute-force computational approach by resorting to the nonhydrostatic equations, but this would require a zeta-flop computer….

"The new challenge to applied mathematics and computing for global climate change is to formulate new equations, new models, and new numerical techniques that, when used in concert, self-consistently compute the feedback between the small scales and the climate scales."

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MORE EPISIMS (Cont'd from P. 2.)

In addition, Smith has done interviews for the Discover Channel and for the Canadian Broadcast Channel (Canada's equivalent to the Public Broadcasting System).

Smith said he learned some interesting things about television because of his recent interview experiences. For Discover, he said, John Bass in the Laboratory Public Affairs Office gave him good advice about clothing and then set him up with good lighting and a camera—but the interviewer called in by telephone from Canada. Smith has no way of knowing when the interview will appear, but when it does, "It will look like a live interview" with Smith and the interviewer in the same room. "We went through this, redoing the whole interview, about five times," he said. The entire process took about an hour, but when the interview appears, it will probably be only five minutes long.

The Canadian Broadcast Channel interviewed him to gather background information for a long show that is in preparation now.

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In Case You Missed It….

Computer and Computational Sciences Division Leader William J. Feiereisen noted during his April 7 All-Hands Meeting that CCS staff members made a major contribution to the latest issue of Los Alamos Science. He said:

"As most of you know, the latest issue of Los Alamos Science is out (volume 5). In it, you will find many interesting articles highlighting technical activities around science-based prediction for complex systems. Included in the issue are four articles authored or co-authored by CCS Division staff. These are:

"'Error Analysis and Simulations of Complex Phenomena,' John Grove, CCS-2, co-author;

"'The LANS-alpha Model for Computing Turbulence—Origins, Results, and Open Problems,' Darryl Holm, CCS-2, Daniel Livescu, CCS-2, Beth Wingate, CCS-2, co-authors;

"'Taylor's Hypothesis, Hamilton's Principle, and the LANS-alpha Model for Computing Turbulence,' Darryl Holm, CCS-2, author; and

"'Physically Motivated Discretization Methods—A Strategy for Increased Predictiveness,' Jim Morel, CCS-2, co-author."

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